

New rigorous perturbation bounds for the LU and QR factorizations

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SUMMARY

Combining the modified matrix-vector equation approach with the technique of Lyapunov majorant function and the Banach fixed point principle, we obtain new rigorous perturbation bounds for the LU and QR factorizations with normwise or componentwise perturbations in the given matrix, where the componentwise perturbations have the form of backward errors resulting from the standard factorization algorithms. Each of the new rigorous perturbation bounds is a rigorous version of the first-order perturbation bound derived by the matrix-vector equation approach in the literature, and we present their explicit expressions. These bounds improve the results given by Chang and Stehlé [*SIAM Journal on Matrix Analysis and Applications* 2010; 31:2841–2859]. Moreover, we derive new tighter first-order perturbation bounds including two optimal ones for the LU factorization, and provide the explicit expressions of the optimal first-order perturbation bounds for the LU and QR factorizations.

KEY WORDS: LU factorization; QR factorization; Lyapunov majorant function; Banach fixed point principle; rigorous perturbation bound; first-order perturbation bound

1. INTRODUCTION

Let $\mathbb{R}^{m \times n}$ be the set of $m \times n$ real matrices and $\mathbb{R}_r^{m \times n}$ be the subset of $\mathbb{R}^{m \times n}$ with rank r . Let I_r be the identity matrix of order r and A^T be the transpose of the matrix A .

For a matrix $A \in \mathbb{R}^{n \times n}$, if its leading principal sub-matrices are all nonsingular, then there exists a unique unit lower triangular matrix $L \in \mathbb{R}^{n \times n}$ and a unique upper triangular matrix $U \in \mathbb{R}^{n \times n}$ such that

$$A = LU. \quad (1.1)$$

The factorization is called the LU factorization of the matrix A , and the matrices L and U are referred to as the LU factors. The LU factorization is a basic and effective tool in numerical linear algebra (see e.g., [1, 2]).

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For a matrix $A \in \mathbb{R}_n^{m \times n}$, there exists a unique matrix $Q \in \mathbb{R}^{m \times n}$ with orthonormal columns, i.e., $Q^T Q = I_n$, and a unique upper triangular matrix $R \in \mathbb{R}^{n \times n}$ with positive diagonal elements such that

$$A = QR. \quad (1.2)$$

The factorization is called the QR factorization of the matrix A , and the matrices Q and R are named after the orthonormal factor and the triangular factor, respectively. The QR factorization is an important tool in matrix computations (see e.g., [1, 2]).

For the LU and QR factorizations, their applications, algorithms, and stability of algorithms have been considered (see e.g., [1, 2, 3]). Since the object matrix A may be contaminated by the errors from measurement, modeling, and so on, and the numerical algorithms will introduce rounding errors in computing these factorizations, the computed factors may not be the exact ones. Naturally, it is important to know how much the factors may change when the original matrix changes. Therefore, several scholars discussed the perturbation analysis of the LU and QR factorizations. The first rigorous perturbation bounds for the LU factorization was derived by Barrlund [4] when the original matrix has the normwise perturbation. Here, a bound is said to be *rigorous* if it doesn't neglect any higher-order terms. Later, using a different approach, Stewart [5] presented the first-order perturbation bounds. These results were improved in [6]. For the QR factorization, the first rigorous perturbation bounds with normwise perturbation were given in [7], which were further modified and improved by Sun [8]. Sun [8] also provided the first-order perturbation bounds, which were obtained by Stewart [5] too using a different approach. Later, Sun [9] presented new rigorous perturbation bounds for the orthonormal factor Q alone, from which an improved first-order perturbation bound was derived. This bound was also given in [10].

In 1996, Chang *et al.* [11] proposed the refined matrix equation approach and the matrix-vector equation approach, which can be used to apply the first-order perturbation analysis of many matrix factorizations, such as, the Cholesky, LU, QR, and SR factorizations [11, 12, 13, 14, 15, 16, 17, 18, 19], when the original matrix has normwise or componentwise perturbations. Here, the componentwise perturbations have the form of backward errors for the standard factorization algorithms (see e.g., [3]). This class of perturbations was first investigated by Zha [20] for the QR factorization. The new first-order perturbation bounds with the above two approaches improve the previous ones greatly. Recently, a new approach, the combination of the classic and refined matrix equation approaches, was provided by Chang *et al.* to study the rigorous perturbation bounds for some matrix factorizations [21, 22, 23, 24]. With their approach, the new rigorous perturbation bounds can be much smaller than the previous ones derived by the classic matrix equation approach. In addition, the rigorous perturbation bounds for the Cholesky factorization can also be obtained by combining the matrix-vector equation approach and the results in [25, Theorem 3.1]; the reader can refer to [11] or [12]. These bounds are tighter than the ones in [23]. However, the above technique can not be applied to the LU factorization. The main reason is that Theorem 3.1 in [25] can not be used any longer. Furthermore, the rigorous bounds derived by the above technique have no explicit expressions and then it is difficult to interpret and understand them.

In this paper, we combine the modified matrix-vector equation approach, the technique of Lyapunov majorant function (see, e.g., [26, Chapter 5]), and the Banach fixed point principle (see, e.g., [26, Appendix D]) to investigate the rigorous perturbation bounds for the LU factorization. Moreover, the rigorous perturbation bounds for the triangular factor R of the QR factorization are also obtained by using the above approach. The new bounds for the LU and QR factorizations can be regarded as the rigorous versions of the first-order perturbation bounds derived by the matrix-vector equation approach in [12], [16], [18], and [19], have the explicit expressions, and improve the corresponding ones in [23]

and [24].

The rest of this paper is organized as follows. Section 2 presents some notation and preliminaries. The rigorous perturbation bounds for the LU and QR factorizations with normwise or componentwise perturbations are given in Sections 3 and 4, respectively. In particular, new tighter first-order perturbation bounds for the LU factorization and the explicit expressions of the optimal first-order perturbation bounds for the LU and QR factorizations are also provided in these two sections. Finally, we present the concluding remarks of the whole paper.

2. NOTATION AND PRELIMINARIES

Given the matrix $A = (a_{ij}) \in \mathbb{R}^{m \times n}$, the symbols A^\dagger , $\|A\|_2$, and $\|A\|_F$ stand for its Moore-Penrose inverse (see, e.g., [27, Chapter III]), spectral norm, and Frobenius norm, respectively, $\kappa_2(A) = \|A^\dagger\|_2 \|A\|_2$ denotes its condition number, and $|A|$ is defined by $|A| = (|a_{ij}|)$. For the above two norms, the following relations hold (see, e.g., [27, page 80]),

$$\|XYZ\|_F \leq \|X\|_2 \|Y\|_F \|Z\|_2, \quad \|XYZ\|_2 \leq \|X\|_2 \|Y\|_2 \|Z\|_2, \quad (2.1)$$

whenever the matrix product XYZ is defined. Note that the Frobenius norm is monotone (see, e.g., [2, Chapter 6]). That is, for a matrix $B = (b_{ij}) \in \mathbb{R}^{m \times n}$, if $|A| \leq |B|$, then $\|A\|_F = \| |A| \|_F \leq \| |B| \|_F = \|B\|_F$. Here $A \leq B$ means $a_{ij} \leq b_{ij}$ for each $i = 1, 2, \dots, m$, $j = 1, 2, \dots, n$. In addition, for a matrix 2-tuple $C = \begin{bmatrix} A \\ B \end{bmatrix}$, we define the ‘generalized matrix norm’ (see, e.g., [26, page 13]) by

$$|||C||| = \begin{bmatrix} \|A\|_F \\ \|B\|_F \end{bmatrix}. \quad (2.2)$$

For the matrix $A = [a_1, a_2, \dots, a_n] = (a_{ij}) \in \mathbb{R}^{n \times n}$, we denote the vector of the first i elements of a_j by $a_j^{(i)}$ and the vector of the last i elements of a_j by $a_j^{[i]}$. With these, we adopt the operators as in [12],

$$\begin{aligned} \text{uvec}(A) &:= \begin{bmatrix} a_1^{(1)} \\ a_2^{(2)} \\ \vdots \\ a_n^{(n)} \end{bmatrix} \in \mathbb{R}^{v_1}, \quad \text{slvec}(A) := \begin{bmatrix} a_1^{[n-1]} \\ a_2^{[n-2]} \\ \vdots \\ a_{n-1}^{[1]} \end{bmatrix} \in \mathbb{R}^{v_2}, \quad \text{vec}(A) := \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} \in \mathbb{R}^{n^2}, \\ \text{up}(A) &:= \begin{bmatrix} \frac{1}{2}a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & \frac{1}{2}a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{2}a_{nn} \end{bmatrix} \in \mathbb{U}_n, \quad \text{ut}(A) := \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{bmatrix} \in \mathbb{U}_n, \end{aligned}$$

and

$$\text{slt}(A) := A - \text{ut}(A) \in \mathbb{SL}_n,$$

where $v_1 = n(n+1)/2$, $v_2 = n(n-1)/2$, and \mathbb{U}_n and \mathbb{SL}_n denote the sets of $n \times n$ real upper triangular and strictly lower triangular matrices, respectively. Considering the structures of these operators, we have

$$\text{uvec}(A) = M_{\text{uvec}} \text{vec}(A), \quad \text{slvec}(A) = M_{\text{slvec}} \text{vec}(A), \quad (2.3)$$

and

$$\text{vec}(\text{up}(A)) = M_{\text{up}} \text{vec}(A), \text{vec}(\text{ut}(A)) = M_{\text{ut}} \text{vec}(A), \text{vec}(\text{slt}(A)) = M_{\text{slt}} \text{vec}(A), \quad (2.4)$$

where

$$\begin{aligned} M_{\text{uvec}} &= \text{diag}(J_1, J_2, \dots, J_n) \in \mathbb{R}^{v_1 \times n^2}, J_i = [I_i, 0_{i \times (n-i)}] \in \mathbb{R}^{i \times n}, \\ M_{\text{slvec}} &= \left[\text{diag}(\tilde{J}_1, \tilde{J}_2, \dots, \tilde{J}_{n-1}), 0_{v_2 \times n} \right] \in \mathbb{R}^{v_2 \times n^2}, \tilde{J}_i = [0_{(n-i) \times i}, I_{n-i}] \in \mathbb{R}^{(n-i) \times n}, \\ M_{\text{up}} &= \text{diag}(S_1, S_2, \dots, S_n) \in \mathbb{R}^{n^2 \times n^2}, S_i = \text{diag}(I_{i-1}, 1/2, 0_{(n-i) \times (n-i)}) \in \mathbb{R}^{n \times n}, \\ M_{\text{ut}} &= \text{diag}(\tilde{S}_1, \tilde{S}_2, \dots, \tilde{S}_n) \in \mathbb{R}^{n^2 \times n^2}, \tilde{S}_i = \text{diag}(I_i, 0_{(n-i) \times (n-i)}) \in \mathbb{R}^{n \times n}, \\ M_{\text{slt}} &= \text{diag}(\hat{S}_1, \hat{S}_2, \dots, \hat{S}_{n-1}, 0_{n \times n}) \in \mathbb{R}^{n^2 \times n^2}, \hat{S}_i = \text{diag}(0_{i \times i}, I_{n-i}) \in \mathbb{R}^{n \times n}. \end{aligned}$$

Here, $0_{s \times t}$ is the $s \times t$ zero matrix. It is easy to verify that

$$M_{\text{uvec}} M_{\text{uvec}}^T = I_{v_1}, M_{\text{slvec}} M_{\text{slvec}}^T = I_{v_2}, \quad (2.5)$$

and

$$M_{\text{uvec}}^T M_{\text{uvec}} = M_{\text{ut}}, M_{\text{slvec}}^T M_{\text{slvec}} = M_{\text{slt}}. \quad (2.6)$$

Let $\text{uvec}^\dagger : \mathbb{R}^{v_1} \rightarrow \mathbb{R}^{n \times n}$ be the right inverse of the operator ‘uvec’ such that $\text{uvec} \cdot \text{uvec}^\dagger = 1_{v_1 \times v_1}$ and $\text{uvec}^\dagger \cdot \text{uvec} = \text{ut}$. Then the matrix of the operator ‘uvec[†]’ is M_{uvec}^T . That is, $\text{uvec}^\dagger(A) = M_{\text{uvec}}^T \text{vec}(A)$. Similarly, we can define the right inverse of the operator ‘slvec’ by ‘slvec[†]’, whose matrix is M_{slvec}^T . Some results mentioned above can be found in [28].

Let $A = (a_{ij}) \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{p \times q}$. The *Kronecker product* between A and B is defined by (see, e.g., [29, Chapter 4]),

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \cdots & a_{1n}B \\ a_{21}B & a_{22}B & \cdots & a_{2n}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}B & a_{m2}B & \cdots & a_{mn}B \end{bmatrix} \in \mathbb{R}^{mp \times nq}.$$

It follows from [29, Chapter 4] that

$$\text{vec}(AXB) = (B^T \otimes A) \text{vec}(X) \quad (2.7)$$

and

$$\Pi_{mn} \text{vec}(A) = \text{vec}(A^T), \quad (2.8)$$

where $X \in \mathbb{R}^{n \times p}$, and $\Pi_{mn} \in \mathbb{R}^{mn \times mn}$ is called the *vec-permutation matrix* and can be expressed explicitly by

$$\Pi_{mn} = \sum_{i=1}^n \sum_{j=1}^m E_{ij}(m \times n) \otimes E_{ji}(n \times m).$$

In the above expression, $E_{ij}(m \times n) = e_i(m)(e_j(n))^T \in \mathbb{R}^{m \times n}$ denotes the (i, j) -th elementary matrix and $e_i(m)$ is the vector $[0, 0, \dots, 0, 1, 0, 0, \dots, 0]^T \in \mathbb{R}^m$, i.e., the 1 in the i -th component. In addition, from [29, Chapter 4], we also have that if A and B are nonsingular, then $A \otimes B$ is also nonsingular and

$$(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}. \quad (2.9)$$

3. PERTURBATION BOUNDS FOR THE LU FACTORIZATION

Assume that the matrices A , L , and U in (1.1) are perturbed as

$$A \rightarrow A + \Delta A, \quad L \rightarrow L + \Delta L, \quad U \rightarrow U + \Delta U,$$

where $\Delta A \in \mathbb{R}^{n \times n}$, $\Delta L \in \mathbb{S}\mathbb{L}_n$, and $\Delta U \in \mathbb{U}_n$. Then the perturbed LU factorization of A is

$$A + \Delta A = (L + \Delta L)(U + \Delta U). \quad (3.1)$$

In the following, we regard the perturbations ΔL and ΔU as the unknown matrices of the matrix equation (3.1), and obtain the condition under which the equation (3.1) has the unique solution.

Considering $A = LU$, Eqn. (3.1) can be simplified as

$$L(\Delta U) + (\Delta L)U = \Delta A - (\Delta L)(\Delta U). \quad (3.2)$$

Premultiplying (3.2) by L^{-1} and postmultiplying it by U^{-1} gives

$$(\Delta U)U^{-1} + L^{-1}(\Delta L) = L^{-1}[\Delta A - (\Delta L)(\Delta U)]U^{-1}.$$

Since $L^{-1}(\Delta L)$ is strictly lower triangular and $(\Delta U)U^{-1}$ is upper triangular, we have

$$L^{-1}(\Delta L) = \text{slt} \left(L^{-1}[\Delta A - (\Delta L)(\Delta U)]U^{-1} \right), \quad (3.3)$$

$$(\Delta U)U^{-1} = \text{ut} \left(L^{-1}[\Delta A - (\Delta L)(\Delta U)]U^{-1} \right). \quad (3.4)$$

Let U_{n-1} denote the sub-matrix of U consisting of the first $n-1$ rows and the first $n-1$ columns, and write $U = \begin{bmatrix} U_{n-1} & u \\ 0 & u_{nn} \end{bmatrix}$. Thus, from (3.3), considering the definition of ‘slt,’ it follows that

$$L^{-1}(\Delta L) = \text{slt} \left(L^{-1}[\Delta A - (\Delta L)(\Delta U)] \begin{bmatrix} U_{n-1}^{-1} & 0 \\ 0 & 0 \end{bmatrix} \right).$$

Applying the operator ‘vec’ to the above equation and using (2.7) and (2.4) implies

$$(I_n \otimes L^{-1})\text{vec}(\Delta L) = M_{\text{slt}} \left(\begin{bmatrix} U_{n-1}^{-T} & 0 \\ 0 & 0 \end{bmatrix} \otimes L^{-1} \right) \text{vec}[\Delta A - (\Delta L)(\Delta U)].$$

Premultiplying the above equation by $I_n \otimes L$ and noting (2.9), we get

$$\text{vec}(\Delta L) = (I_n \otimes L)M_{\text{slt}} \left(\begin{bmatrix} U_{n-1}^{-T} & 0 \\ 0 & 0 \end{bmatrix} \otimes L^{-1} \right) \text{vec}[\Delta A - (\Delta L)(\Delta U)]. \quad (3.5)$$

Noticing the structure of ΔL , from (2.4), (2.6), and (2.3), it is seen that

$$\text{vec}(\Delta L) = \text{vec}(\text{slt}(\Delta L)) = M_{\text{slt}}\text{vec}(\Delta L) = M_{\text{slvec}}^T M_{\text{slvec}}\text{vec}(\Delta L) = M_{\text{slvec}}^T \text{slvec}(\Delta L). \quad (3.6)$$

Substituting the above equality into (3.5) and then left-multiplying it by M_{slvec} and using (2.5) yields

$$\text{slvec}(\Delta L) = M_{\text{slvec}}(I_n \otimes L)M_{\text{slt}} \left(\begin{bmatrix} U_{n-1}^{-T} & 0 \\ 0 & 0 \end{bmatrix} \otimes L^{-1} \right) \text{vec}[\Delta A - (\Delta L)(\Delta U)]. \quad (3.7)$$

Multiplying both sides of (3.7) from the left by M_{slvec}^T and noting (3.6) and (2.6) leads to

$$\text{vec}(\Delta L) = M_{\text{slt}}(I_n \otimes L)M_{\text{slt}} \left(\begin{bmatrix} U_{n-1}^{-T} & 0 \\ 0 & 0 \end{bmatrix} \otimes L^{-1} \right) \text{vec}[\Delta A - (\Delta L)(\Delta U)]. \quad (3.8)$$

From the structure of the matrix M_{slt} , we can verify that $M_{\text{slt}}(I_n \otimes L)M_{\text{slt}} = (I_n \otimes L)M_{\text{slt}}$, which together with (3.8) gives (3.5). Thus, the equations (3.5) and (3.7) are equivalent.

Similarly, applying the operator ‘vec’ to (3.4) and using (2.7), (2.4), and (2.9), we have

$$\text{vec}(\Delta U) = (U^T \otimes I_n) M_{\text{ut}} (U^{-T} \otimes L^{-1}) \text{vec}[\Delta A - (\Delta L)(\Delta U)]. \quad (3.9)$$

It follows from the structure of ΔU , (2.4), (2.6), and (2.3) that

$$\text{vec}(\Delta U) = \text{vec}(\text{ut}(\Delta U)) = M_{\text{ut}} \text{vec}(\Delta U) = M_{\text{uvec}}^T M_{\text{uvec}} \text{vec}(\Delta U) = M_{\text{uvec}}^T \text{uvec}(\Delta U). \quad (3.10)$$

Thus, (3.9), (3.10), and (2.5) together implies

$$\text{uvec}(\Delta U) = M_{\text{uvec}} (U^T \otimes I_n) M_{\text{ut}} (U^{-T} \otimes L^{-1}) \text{vec}[\Delta A - (\Delta L)(\Delta U)]. \quad (3.11)$$

Similar to the discussion for ΔL , from (3.11), considering (3.10), (2.6), and the fact $M_{\text{ut}}(U^T \otimes I_n)M_{\text{ut}} = (U^T \otimes I_n)M_{\text{ut}}$, we get (3.9). So the equations (3.9) and (3.11) are equivalent.

Applying the operators ‘slvec † ’ and ‘uvec † ’ to (3.7) and (3.11), respectively, gives

$$\Delta L = \text{slvec}^\dagger \left(Y_L \text{vec}[\Delta A - (\Delta L)(\Delta U)] \right), \quad (3.12)$$

and

$$\Delta U = \text{uvec}^\dagger \left(Y_U \text{vec}[\Delta A - (\Delta L)(\Delta U)] \right), \quad (3.13)$$

where

$$Y_L = M_{\text{slvec}}(I_n \otimes L)M_{\text{slt}} \left(\begin{bmatrix} U_{n-1}^{-T} & 0 \\ 0 & 0 \end{bmatrix} \otimes L^{-1} \right), \quad Y_U = M_{\text{uvec}}(U^T \otimes I_n)M_{\text{ut}}(U^{-T} \otimes L^{-1}).$$

The matrices Y_L and Y_U are just the ones in [16, Eqn. (3.5)], where their explicit expressions are not given. This fact can be obtained from (3.7) and (3.11), and [16, Eqn. (3.6)] by setting $t = \varepsilon$ in [16, Eqn. (3.6)] and dropping the higher-order terms.

Now we apply the technique of Lyapunov majorant function and the Banach fixed point principle to derive the rigorous perturbation bounds for ΔL and ΔU on the basis of (3.12) and (3.13).

Let $\Delta X = \begin{bmatrix} \Delta L \\ \Delta U \end{bmatrix}$. Then the equations (3.12) and (3.13) can be rewritten as an operator equation for ΔX ,

$$\Delta X = \Phi(\Delta X, \Delta A) = \begin{bmatrix} \Phi_1(\Delta X, \Delta A) \\ \Phi_2(\Delta X, \Delta A) \end{bmatrix}, \quad (3.14)$$

where $\Phi_1(\Delta X, \Delta A) = \text{slvec}^\dagger \left(Y_L \text{vec}[\Delta A - (\Delta L)(\Delta U)] \right)$ and $\Phi_2(\Delta X, \Delta A) = \text{uvec}^\dagger \left(Y_U \text{vec}[\Delta A - (\Delta L)(\Delta U)] \right)$. Assume that $Z_1 \in \mathbb{S}\mathbb{L}_n$, $Z_2 \in \mathbb{U}_n$, and $Z = \begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix}$. Replacing ΔX in (3.14) with Z gives

$$Z = \Phi(Z, \Delta A) = \begin{bmatrix} \Phi_1(Z, \Delta A) \\ \Phi_2(Z, \Delta A) \end{bmatrix}, \quad (3.15)$$

where $\Phi_1(Z, \Delta A)$ and $\Phi_2(Z, \Delta A)$ are the same as $\Phi_1(\Delta X, \Delta A)$ and $\Phi_2(\Delta X, \Delta A)$, respectively, with ΔX being replaced by Z . Let $\|Z\| \leq \rho = \begin{bmatrix} \rho_1 \\ \rho_2 \end{bmatrix}$, i.e., $\|Z_1\|_F \leq \rho_1$ and $\|Z_2\|_F \leq \rho_2$ for some $\rho_1 \geq 0$ and

$\rho_2 \geq 0$, and $\|\Delta A\|_F = \delta$. Then it follows from the definitions of the ‘generalized matrix norm’ (2.2) and the operators ‘uvec[†]’ and ‘slvec[†]’, with (2.1), that

$$|||\Phi(Z, \Delta A)||| = \begin{bmatrix} \|\Phi_1(Z, \Delta A)\|_F \\ \|\Phi_2(Z, \Delta A)\|_F \end{bmatrix} \leq \begin{bmatrix} \|Y_L\|_2 (\delta + \rho_1 \rho_2) \\ \|Y_U\|_2 (\delta + \rho_1 \rho_2) \end{bmatrix}.$$

Thus, we have the Lyapunov majorant function (see, e.g., [26, Chapter 5]) of the operator equation (3.15)

$$h(\rho, \delta) = \begin{bmatrix} h_1(\rho, \delta) \\ h_2(\rho, \delta) \end{bmatrix} = \begin{bmatrix} \|Y_L\|_2 (\delta + \rho_1 \rho_2) \\ \|Y_U\|_2 (\delta + \rho_1 \rho_2) \end{bmatrix},$$

and the Lyapunov majorant equation (see, e.g., [26, Chapter 5])

$$h(\rho, \delta) = \rho, \text{ i.e., } \begin{cases} \|Y_L\|_2 (\delta + \rho_1 \rho_2) = \rho_1, \\ \|Y_U\|_2 (\delta + \rho_1 \rho_2) = \rho_2. \end{cases}$$

Then

$$\rho_2 = \frac{\|Y_U\|_2}{\|Y_L\|_2} \rho_1, \quad (3.16)$$

and

$$\|Y_U\|_2 \rho_1^2 - \rho_1 + \|Y_L\|_2 \delta = 0. \quad (3.17)$$

Assume that $\delta \in \Omega = \{\delta \geq 0 : 1 - 4\|Y_U\|_2 \|Y_L\|_2 \delta \geq 0\}$. Then, the Lyapunov majorant equation (3.17) has two nonnegative roots: $\rho_{1,1}(\delta) \leq \rho_{1,2}(\delta)$ with

$$\rho_{1,1}(\delta) := f_1(\delta) := \frac{2\|Y_L\|_2 \delta}{1 + \sqrt{1 - 4\|Y_U\|_2 \|Y_L\|_2 \delta}},$$

which combined with (3.16) gives: $\rho_{2,1}(\delta) \leq \rho_{2,2}(\delta)$ and

$$\rho_{2,1}(\delta) := f_2(\delta) := \frac{2\|Y_U\|_2 \delta}{1 + \sqrt{1 - 4\|Y_U\|_2 \|Y_L\|_2 \delta}}.$$

Let the set $\mathcal{B}(\delta)$ be defined by

$$\mathcal{B}(\delta) = \left\{ Z = \begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix}, Z_1 \in \mathbb{S}\mathbb{L}_n, Z_2 \in \mathbb{U}_n : |||Z||| \leq \begin{bmatrix} f_1(\delta) \\ f_2(\delta) \end{bmatrix} \right\} \subset \mathbb{R}^{2n \times n},$$

which is closed and convex. Thus, the operator $\Phi(\cdot, \Delta A)$ maps the set $\mathcal{B}(\delta)$ into itself. Furthermore, note that the Jacobi matrix of $h(\rho, \delta)$ relative to ρ at ρ_0 is,

$$h'_p(\rho_0, \delta) = \frac{1 - \sqrt{1 - 4\|Y_U\|_2 \|Y_L\|_2 \delta}}{2} \begin{bmatrix} 1 & \|Y_L\|_2 / \|Y_U\|_2 \\ \|Y_U\|_2 / \|Y_L\|_2 & 1 \end{bmatrix},$$

where $\rho_0 = \begin{bmatrix} f_1(\delta) \\ f_2(\delta) \end{bmatrix}$, and for $Z, \tilde{Z} \in \mathcal{B}(\delta)$,

$$|||\Phi(Z, \Delta A) - \Phi(\tilde{Z}, \Delta A)||| \leq h'_p(\rho_0, \delta) |||Z - \tilde{Z}|||.$$

Then if $\delta \in \Omega_1 = \{\delta \geq 0 : 1 - 4\|Y_U\|_2\|Y_L\|_2\delta > 0\}$, we have that the spectral radius of $h'_\rho(\rho_0, \delta)$ is smaller than 1 and then the operator $\Phi(\cdot, \Delta A)$ is generalized contractive (see, e.g., [26, Appendix D]) on $\mathcal{B}(\delta)$. According to the generalized Banach fixed point principle (see, e.g., [26, Appendix D]), there exists a unique solution to the operator equation (3.15) in the set $\mathcal{B}(\delta)$ when $\delta \in \Omega_1$, and so does the operator equation (3.14). As a result, we have

$$\|\Delta X\| \leq \begin{bmatrix} f_1(\delta) \\ f_2(\delta) \end{bmatrix}, \quad \delta \in \Omega_1.$$

Considering the equivalence of the matrix equation (3.1) and the operator equation (3.14), we have the main theorem.

Theorem 3.1. *Let the unique LU factorization of $A \in \mathbb{R}_n^{n \times n}$ be as in (1.1) and $\Delta A \in \mathbb{R}^{n \times n}$. If*

$$\|Y_L\|_2\|Y_U\|_2\|\Delta A\|_F < \frac{1}{4}, \quad (3.18)$$

then $A + \Delta A$ has the unique LU factorization (3.1). Moreover,

$$\|\Delta L\|_F \leq \frac{2\|Y_L\|_2\|\Delta A\|_F}{1 + \sqrt{1 - 4\|Y_U\|_2\|Y_L\|_2\|\Delta A\|_F}} \quad (3.19)$$

$$\leq 2\|Y_L\|_2\|\Delta A\|_F \quad (3.20)$$

$$= 2\left\|(I_n \otimes L)M_{\text{slt}}\left(\begin{bmatrix} U_{n-1}^{-T} & 0 \\ 0 & 0 \end{bmatrix} \otimes L^{-1}\right)\right\|_2\|\Delta A\|_F, \quad (3.21)$$

and

$$\|\Delta U\|_F \leq \frac{2\|Y_U\|_2\|\Delta A\|_F}{1 + \sqrt{1 - 4\|Y_U\|_2\|Y_L\|_2\|\Delta A\|_F}} \quad (3.22)$$

$$\leq 2\|Y_U\|_2\|\Delta A\|_F \quad (3.23)$$

$$= 2\|(U^T \otimes I_n)M_{\text{ut}}(U^{-T} \otimes L^{-1})\|_2\|\Delta A\|_F. \quad (3.24)$$

Proof. From the discussions before Theorem 3.1, we only need to show that (3.21) and (3.24) hold. Considering the definition of the spectral norm, (2.6), and the facts

$$M_{\text{slt}}(I_n \otimes L)M_{\text{slt}} = (I_n \otimes L)M_{\text{slt}}, \quad M_{\text{ut}}(U^T \otimes I_n)M_{\text{ut}} = (U^T \otimes I_n)M_{\text{ut}}, \quad (3.25)$$

it is easy to verify that

$$\|Y_L\|_2 = \left\|(I_n \otimes L)M_{\text{slt}}\left(\begin{bmatrix} U_{n-1}^{-T} & 0 \\ 0 & 0 \end{bmatrix} \otimes L^{-1}\right)\right\|_2, \quad \|Y_U\|_2 = \|(U^T \otimes I_n)M_{\text{ut}}(U^{-T} \otimes L^{-1})\|_2.$$

So (3.21) and (3.24) hold. \square

Remark 3.1. From (3.19) and (3.22), we have the following first-order perturbation bounds,

$$\|\Delta L\|_F \leq \left\|(I_n \otimes L)M_{\text{slt}}\left(\begin{bmatrix} U_{n-1}^{-T} & 0 \\ 0 & 0 \end{bmatrix} \otimes L^{-1}\right)\right\|_2\|\Delta A\|_F + \mathcal{O}(\|\Delta A\|_F^2), \quad (3.26)$$

and

$$\|\Delta U\|_F \leq \|(U^T \otimes I_n)M_{\text{ut}}(U^{-T} \otimes L^{-1})\|_2\|\Delta A\|_F + \mathcal{O}(\|\Delta A\|_F^2). \quad (3.27)$$

Note that, in this case, the condition (3.18) can be weakened to

$$\|L^{-1}\|_2 \|U^{-1}\|_2 \|\Delta A\|_F < 1. \quad (3.28)$$

This is because the bounds (3.26) and (3.27) can be derived from (3.12) and (3.13) directly by omitting the higher-order terms. We only provide the condition under which the LU factorization of $A + \Delta A$ exists and is unique. From [23, Proof of Theorem 4.1], it follows that the condition (3.28) is enough.

The bounds (3.26) and (3.27) without explicit expressions were also derived by the matrix-vector equation approach in [16], which are considered to be optimal.

Remark 3.2. The rigorous perturbation bounds derived by the combination of the classic and refined matrix equation approaches presented in [23] are as follows,

$$\|\Delta L\|_F \leq 2 \left(\inf_{D_L \in \mathbb{D}_n} k_2(LD_L^{-1}) \right) \|U_{n-1}^{-1}\|_2 \|\Delta A\|_F, \quad (3.29)$$

and

$$\|\Delta U\|_F \leq 2 \left(\inf_{D_U \in \mathbb{D}_n} k_2(D_U^{-1}U) \right) \|L^{-1}\|_2 \|\Delta A\|_F, \quad (3.30)$$

under the condition

$$\|L^{-1}\|_2 \|U^{-1}\|_2 \|\Delta A\|_F < 1/4. \quad (3.31)$$

In (3.29) and (3.30), \mathbb{D}_n denotes the set of $n \times n$ positive definite diagonal matrices. The bounds (3.29) and (3.30) can be much smaller than the previous ones derived by the classic matrix equation approach; see discussions in [23]. From [16, Eqns. (3.17) and (3.24)], we have

$$\|Y_L\|_2 \leq \left(\inf_{D_L \in \mathbb{D}_n} k_2(LD_L^{-1}) \right) \|U_{n-1}^{-1}\|_2, \quad \|Y_U\|_2 \leq \left(\inf_{D_U \in \mathbb{D}_n} k_2(D_U^{-1}U) \right) \|L^{-1}\|_2.$$

So the bounds (3.21) and (3.24) are tighter than (3.29) and (3.30), respectively. Unfortunately, it follows from [16, Eqns. (3.18) and (3.25)] that

$$\|Y_L\|_2 \geq \|U_{n-1}^{-1}\|_2, \quad \|Y_U\|_2 \geq \|L^{-1}\|_2.$$

Thus, the condition (3.18) is more constraining than (3.31). Fortunately, the above two lower bounds are attainable [12, 16], which shows that the condition (3.18) is not so constraining. In addition, it is also a little more expensive to estimate the bounds (3.21) and (3.24) than that of (3.29) and (3.30) because the former involves the Kronecker products. These should be the price of having tighter rigorous perturbation results.

Considering the standard techniques of backward error analysis (see, e.g., [2, Theorem 9.3]), we have that the computed LU factors \tilde{L} and \tilde{U} by the Gaussian elimination satisfy,

$$\tilde{A} = A + \Delta A = \tilde{L}\tilde{U}, \quad |\Delta A| \leq \varepsilon |\tilde{L}||\tilde{U}|, \quad (3.32)$$

where $\varepsilon = n\mathbf{u}/(1 - n\mathbf{u})$ with \mathbf{u} being the unit roundoff. In the following, we consider the rigorous perturbation bounds for the LU factorization with the perturbation ΔA having the same form as in (3.32). The new bounds, similar to the ones in [23], will involve the LU factors of \tilde{A} . The reader can refer to [23, Section 4] for an explanation.

Assume that the matrices \tilde{A} , \tilde{L} , and \tilde{U} in (3.32) are perturbed as

$$\tilde{A} \rightarrow \tilde{A} - \Delta A, \quad \tilde{L} \rightarrow \tilde{L} - \Delta L, \quad \tilde{U} \rightarrow \tilde{U} - \Delta U,$$

where $\Delta A \in \mathbb{R}^{n \times n}$ is as in (3.32), $\Delta L \in \mathbb{SL}_n$, and $\Delta U \in \mathbb{U}_n$. Then the perturbed LU factorization of \tilde{A} is

$$A = \tilde{A} - \Delta A = (\tilde{L} - \Delta L)(\tilde{U} - \Delta U),$$

which together with (3.32) yields,

$$\tilde{L}(\Delta U) + (\Delta L)\tilde{U} = \Delta A + (\Delta L)(\Delta U).$$

As done before, we regard the perturbations ΔL and ΔU as the unknown matrices. Thus, similar to the induction before Theorem 3.1, replacing L and U with \tilde{L} and \tilde{U} , respectively, we have

$$\Delta X = \tilde{\Phi}(\Delta X, \Delta A) = \begin{bmatrix} \tilde{\Phi}_1(\Delta X, \Delta A) \\ \tilde{\Phi}_2(\Delta X, \Delta A) \end{bmatrix}, \quad (3.33)$$

where

$$\tilde{\Phi}_1(\Delta X, \Delta A) = \text{svec}^\dagger \left(Y_{\tilde{L}} \text{vec}(\Delta A) + Y_{\tilde{L}} \text{vec}[(\Delta L)(\Delta U)] \right) \quad (3.34)$$

and

$$\tilde{\Phi}_2(\Delta X, \Delta A) = \text{uvec}^\dagger \left(Y_{\tilde{U}} \text{vec}(\Delta A) + Y_{\tilde{U}} \text{vec}[(\Delta L)(\Delta U)] \right). \quad (3.35)$$

Here

$$Y_{\tilde{L}} = M_{\text{svec}} \left(I_n \otimes \tilde{L} \right) M_{\text{slt}} \left(\begin{bmatrix} \tilde{U}_{n-1}^{-T} & 0 \\ 0 & 0 \end{bmatrix} \otimes \tilde{L}^{-1} \right), \quad Y_{\tilde{U}} = M_{\text{uvec}} \left(\tilde{U}^T \otimes I_n \right) M_{\text{ut}} \left(\tilde{U}^{-T} \otimes \tilde{L}^{-1} \right).$$

Considering (3.32), the fact that the Frobenius norm is monotone, and (2.1), we obtain

$$\left\| \tilde{\Phi}_1(Z, \Delta A) \right\|_F \leq \left\| |Y_{\tilde{L}}| \text{vec} \left(|\tilde{L}| |\tilde{U}| \right) \right\|_F \varepsilon + \left\| |Y_{\tilde{L}}| \right\|_2 \rho_1 \rho_2$$

and

$$\left\| \tilde{\Phi}_2(Z, \Delta A) \right\|_F \leq \left\| |Y_{\tilde{U}}| \text{vec} \left(|\tilde{L}| |\tilde{U}| \right) \right\|_F \varepsilon + \left\| |Y_{\tilde{U}}| \right\|_2 \rho_1 \rho_2.$$

Similar to the discussions before Theorem 3.1, using the above two inequalities, we have the following theorem.

Theorem 3.2. Assume that $\Delta A \in \mathbb{R}^{n \times n}$ is a perturbation in $A \in \mathbb{R}^{n \times n}$ and $A + \Delta A$ has the unique LU factorization satisfying (3.32). Let $a = \left\| |Y_{\tilde{L}}| \text{vec}(|\tilde{L}| |\tilde{U}|) \right\|_F$, $b = \left\| |Y_{\tilde{U}}| \text{vec}(|\tilde{L}| |\tilde{U}|) \right\|_F$, and $c = b \left\| |Y_{\tilde{L}}| \right\|_2 - a \left\| |Y_{\tilde{U}}| \right\|_2$. If

$$|c| \varepsilon < 1 \quad \text{and} \quad 4a \left\| |Y_{\tilde{U}}| \right\|_2 \varepsilon < (1 - c\varepsilon)^2, \quad (3.36)$$

then A has the unique LU factorization $A = LU$, where $L = \tilde{L} - \Delta L$ and $U = \tilde{U} - \Delta U$. Moreover,

$$\left\| \Delta L \right\|_F \leq \frac{2a\varepsilon}{1 - c\varepsilon + \sqrt{(1 - c\varepsilon)^2 - 4a \left\| |Y_{\tilde{U}}| \right\|_2 \varepsilon}} \quad (3.37)$$

$$\leq \frac{2a\varepsilon}{1 - c\varepsilon}, \quad (3.38)$$

and

$$\|\Delta U\|_F \leq \frac{2b\varepsilon}{1 + c\varepsilon + \sqrt{(1 - c\varepsilon)^2 - 4a\|Y_{\tilde{U}}\|_2\varepsilon}} \quad (3.39)$$

$$\leq \frac{2b\varepsilon}{1 + c\varepsilon}. \quad (3.40)$$

Remark 3.3. From (3.37) and (3.39), we have the following first-order perturbation bounds,

$$\|\Delta L\|_F \leq \|Y_{\tilde{L}}|\text{vec}(|\tilde{L}||\tilde{U}|)\|_F \varepsilon + \mathcal{O}(\varepsilon^2), \quad (3.41)$$

and

$$\|\Delta U\|_F \leq \|Y_{\tilde{U}}|\text{vec}(|\tilde{L}||\tilde{U}|)\|_F \varepsilon + \mathcal{O}(\varepsilon^2), \quad (3.42)$$

which can also be derived from (3.33)–(3.35), and (3.32) directly by omitting the higher-order terms. Therefore, in this case, the condition (3.36) can be weakened to

$$\| \tilde{L}^{-1} \|\tilde{L}\|_F \| \tilde{U} \|\tilde{U}^{-1}\|_F \varepsilon < 1, \quad (3.43)$$

which guarantees that the unique LU factorization of $\tilde{A} - \Delta A = A$ exists [23, Proof of Theorem 4.2]. Using (3.33)–(3.35), and (3.32), we can also obtain the first-order perturbation bounds with respect to the ‘ M ’-norm and the ‘ S ’-norm,

$$\|\Delta L\|_v \leq \|Y_{\tilde{L}}|\text{vec}(|\tilde{L}||\tilde{U}|)\|_v \varepsilon + \mathcal{O}(\varepsilon^2), \quad (3.44)$$

and

$$\|\Delta U\|_v \leq \|Y_{\tilde{U}}|\text{vec}(|\tilde{L}||\tilde{U}|)\|_v \varepsilon + \mathcal{O}(\varepsilon^2), \quad (3.45)$$

where $v = M$ or S , under the condition (3.43). Recall that the M -norm and the S -norm of a matrix $A = (a_{ij}) \in \mathbb{R}^{m \times n}$ are defined by (see, e.g., [2, Chapter 6]),

$$\|A\|_M = \max_{i,j} |a_{ij}|, \quad \|A\|_S = \sum_{i,j} |a_{ij}|,$$

respectively, which are both monotone. For the M -norm, the first-order bound for ΔL , i.e., (3.44), is attained for ΔA satisfying

$$\text{vec}(\Delta A) = \varepsilon D_k \text{vec}(|\tilde{L}||\tilde{U}|), \quad D_k = \text{diag}(\xi_1, \xi_2, \dots, \xi_{n^2}),$$

where $\xi_i = \text{sign}(Y_{\tilde{L}}(k, i))$ and $\|Y_{\tilde{L}}|\text{vec}(|\tilde{L}||\tilde{U}|)\|_M = (Y_{\tilde{L}}|\text{vec}(|\tilde{L}||\tilde{U}|))(k, 1)$. Here, the MATLAB notation is used. If we take $\xi_i = \text{sign}(Y_{\tilde{U}}(k, i))$ and $\|Y_{\tilde{U}}|\text{vec}(|\tilde{L}||\tilde{U}|)\|_M = (Y_{\tilde{U}}|\text{vec}(|\tilde{L}||\tilde{U}|))(k, 1)$, then the first-order bound for ΔU , i.e., (3.45), is attained under the M -norm for this ΔA . Thus, we obtain the optimal first-order perturbation bounds for the LU factorization under the M -norm.

In [15], Chang presented the following first-order perturbation bounds under the consistent and monotone norm $\|\cdot\|$,

$$\|\Delta L\| \leq \left\| |\tilde{L}| \tilde{L}^{-1} |\tilde{L}| \right\| \cdot \left\| |\tilde{U}_{n-1}| |\tilde{U}_{n-1}^{-1}| \right\| \varepsilon + \mathcal{O}(\varepsilon^2), \quad (3.46)$$

and

$$\|\Delta U\| \leq \left\| |\tilde{U}| \tilde{U}^{-1} |\tilde{U}| \right\| \cdot \left\| |\tilde{L}^{-1}| |\tilde{L}| \right\| \varepsilon + \mathcal{O}(\varepsilon^2). \quad (3.47)$$

Since, for the norm $\|\cdot\|_v$ ($v = F$ or S), which are both consistent and monotone, considering (2.7), (2.4), and (2.3), we have

$$\begin{aligned} \left\| |Y_{\tilde{L}}| \text{vec}(|\tilde{L}| |\tilde{U}|) \right\|_v &\leq \left\| M_{\text{svec}}(I_n \otimes |\tilde{L}|) M_{\text{slt}} \left(\begin{bmatrix} |\tilde{U}_{n-1}^{-T}| & 0 \\ 0 & 0 \end{bmatrix} \otimes |\tilde{L}^{-1}| \right) \text{vec}(|\tilde{L}| |\tilde{U}|) \right\|_v \\ &= \left\| \text{svec} \left(|\tilde{L}| \text{slt} \left(|\tilde{L}^{-1}| |\tilde{L}| |\tilde{U}| \begin{bmatrix} |\tilde{U}_{n-1}^{-1}| & 0 \\ 0 & 0 \end{bmatrix} \right) \right) \right\|_v \\ &= \left\| |\tilde{L}| \text{slt} \left(|\tilde{L}^{-1}| |\tilde{L}| |\tilde{U}| \begin{bmatrix} |\tilde{U}_{n-1}^{-1}| & 0 \\ 0 & 0 \end{bmatrix} \right) \right\|_v \\ &\leq \left\| |\tilde{L}| \tilde{L}^{-1} |\tilde{L}| \right\|_v \left\| |\tilde{U}_{n-1}| |\tilde{U}_{n-1}^{-1}| \right\|_v, \end{aligned} \quad (3.48)$$

and

$$\begin{aligned} \left\| |Y_{\tilde{U}}| \text{vec}(|\tilde{L}| |\tilde{U}|) \right\|_v &\leq \left\| M_{\text{uvec}}(|\tilde{U}^T| \otimes I_n) M_{\text{ut}}(|\tilde{U}^{-T}| \otimes |\tilde{L}^{-1}|) \text{vec}(|\tilde{L}| |\tilde{U}|) \right\|_v \\ &= \left\| \text{uvec} \left(\text{ut}(|\tilde{L}^{-1}| |\tilde{L}| |\tilde{U}| |\tilde{U}^{-1}|) |\tilde{U}| \right) \right\|_v \\ &= \left\| \text{ut}(|\tilde{L}^{-1}| |\tilde{L}| |\tilde{U}| |\tilde{U}^{-1}|) |\tilde{U}| \right\|_v \\ &\leq \left\| |\tilde{U}| \tilde{U}^{-1} |\tilde{U}| \right\|_v \left\| |\tilde{L}^{-1}| |\tilde{L}| \right\|_v, \end{aligned} \quad (3.49)$$

the first-order bounds (3.44) and (3.45) are tighter than (3.46) and (3.47) under the two norms, respectively.

In addition, it should be pointed out that we can not achieve the first-order perturbation bounds in terms of the 1-norm and the ∞ -norm, both of which are also consistent and monotone.

Remark 3.4. In [23], the following rigorous perturbation bounds with respect to the consistent and monotone norm were derived by the combination of the classic and refined matrix equation approaches,

$$\|\Delta L\| \leq 2 \left(\inf_{D_L \in \mathbb{D}_n} \left\| \tilde{L} D_L^{-1} \right\| \cdot \left\| D_L |\tilde{L}^{-1}| |\tilde{L}| \right\| \right) \left\| |\tilde{U}_{n-1}| \cdot |\tilde{U}_{n-1}^{-1}| \right\| \varepsilon, \quad (3.50)$$

and

$$\|\Delta U\| \leq 2 \left(\inf_{D_U \in \mathbb{D}_n} \left\| D_U^{-1} \tilde{U} \right\| \cdot \left\| |\tilde{U}| \tilde{U}^{-1} |D_U| \right\| \right) \left\| |\tilde{L}^{-1}| \cdot |\tilde{L}| \right\| \varepsilon, \quad (3.51)$$

under the condition

$$\left\| |\tilde{L}^{-1}| |\tilde{L}| \right\| \cdot \left\| |\tilde{U}| \tilde{U}^{-1} \right\| \varepsilon < 1/4. \quad (3.52)$$

Combining the properties of the operators ‘ut’ and ‘slt’ [23, Eqn (2.5)]

$$\text{slt}(D_L X) = D_L \text{slt}(X), \quad \text{ut}(X D_U) = \text{ut}(X) D_U,$$

where $D_L, D_U \in \mathbb{D}_n$, with (3.48) and (3.49), and noting (2.1), we have

$$\begin{aligned} \left\| |Y_{\tilde{L}}| \text{vec} \left(|\tilde{L}| |\tilde{U}| \right) \right\|_F &\leq \left\| |\tilde{L}| D_L^{-1} \text{slt} \left(D_L |\tilde{L}^{-1}| |\tilde{L}| |\tilde{U}| \begin{bmatrix} |\tilde{U}_{n-1}^{-1}| & 0 \\ 0 & 0 \end{bmatrix} \right) \right\|_F \\ &\leq \left\| |\tilde{L}| D_L^{-1} \right\|_2 \left\| D_L |\tilde{L}^{-1}| |\tilde{L}| \right\|_2 \left\| |\tilde{U}_{n-1}| |\tilde{U}_{n-1}^{-1}| \right\|_F, \end{aligned}$$

and

$$\begin{aligned} \left\| |Y_{\tilde{U}}| \text{vec} \left(|\tilde{L}| |\tilde{U}| \right) \right\|_F &\leq \left\| \text{ut} \left(|\tilde{L}^{-1}| |\tilde{L}| |\tilde{U}| |\tilde{U}^{-1}| D_U \right) D_U^{-1} |\tilde{U}| \right\|_F \\ &\leq \left\| D_U^{-1} |\tilde{U}| \right\|_2 \left\| |\tilde{U}| |\tilde{U}^{-1}| D_U \right\|_2 \left\| |\tilde{L}^{-1}| |\tilde{L}| \right\|_F. \end{aligned}$$

Note that $D_L, D_U \in \mathbb{D}_n$ are arbitrary. Thus, under the Frobenius norm, when

$$\left\| |\tilde{L}| D_L^{-1} \right\|_2 = \left\| \tilde{L} D_L^{-1} \right\|_2, \quad \left\| D_U^{-1} |\tilde{U}| \right\|_2 = \left\| D_U^{-1} \tilde{U} \right\|_2,$$

if $-1 < c\varepsilon < 0$, the bound (3.38) is obviously smaller than (3.50); if $1 > c\varepsilon > 0$, the bound (3.40) is obviously smaller than (3.51); otherwise, the bounds (3.38) and (3.40) are obviously smaller than the corresponding ones (3.50) and (3.51). Notice that for any matrix $X \in \mathbb{R}^{m \times n}$, $\|X\|_2$ is at most $\sqrt{\text{rank}(X)}$ times as large as $\|X\|_F$ (see, e.g., [2, Lemma 6.6]). Especially, the scaling matrices can make $\tilde{L} D_L^{-1}$ and $D_U^{-1} \tilde{U}$ be of special structure. For example, they may have the unit 2-norm columns and rows, respectively. As a result, the differences between $\left\| |\tilde{L}| D_L^{-1} \right\|_2$ and $\left\| \tilde{L} D_L^{-1} \right\|_2$, $\left\| D_U^{-1} |\tilde{U}| \right\|_2$ and $\left\| D_U^{-1} \tilde{U} \right\|_2$ will not be remarkable in general. See the following example. Moreover, since ε is very small, $c\varepsilon$ may also be very small. See Example 3.1 below. Thus, the bounds (3.38) and (3.40) may generally be smaller than (3.50) and (3.51), respectively. An example is given below to indicate this conjecture. However, it should be mentioned that the condition (3.36) is more complicated and may be more constraining than the one (3.52), and it is a slightly more expensive to estimate the bounds in Theorem 3.2.

In addition, we need to point out that we can not obtain the rigorous perturbation bounds under the S -norm, the M -norm, the 1-norm, and the ∞ -norm using the foregoing approach.

Example 3.1. The example is from [16]. That is, each test matrix has the form $A = D_1 B D_2$, where $D_1 = \text{diag}(1, d_1, d_1^2, \dots, d_1^{n-1})$, $D_2 = \text{diag}(1, d_2, d_2^2, \dots, d_2^{n-1})$, and $B \in \mathbb{R}^{n \times n}$ is a random matrix produced by the MATLAB function **randn**. As done in [16], the chosen scaling matrices D_L and D_U are defined by $D_L = \text{diag}(\|L(:, j)\|_2)$ and $D_U = \text{diag}(\|U(j, :)\|_2)$, respectively. Upon computations in MATLAB 7.0 on a PC, with machine precision 2.2×10^{-16} , the numerical results for $n = 10$, $d_1, d_2 \in \{0.2, 1, 2\}$, and the same matrix B are listed in Table 1, which demonstrate the conjectures given in Remark 3.4.

Table 1: Comparison of rigorous bounds for $A = D_1 B D_2$

d_1	d_2	γ_L	$\gamma_L(D_L)$	η_{D_L}	γ_U	$\gamma_U(D_U)$	η_{D_U}	t_γ	$t_{\gamma(D)}$	τ
0.2	0.2	4.31e+01	2.66e+06	1.00	1.00e+00	5.93e+00	1.00	0.007	0.002	9.15e-05
0.2	1	4.31e+01	2.66e+06	1.00	1.38e+00	2.83e+02	1.20	0.009	0.001	6.99e-09
0.2	2	4.31e+01	2.66e+06	1.00	1.49e+00	9.23e+02	1.09	0.026	0.002	5.81e-07
1	0.2	7.17e+01	6.17e+02	1.27	1.03e+00	9.13e+01	1.00	0.010	0.002	2.58e-09
1	1	7.17e+01	6.17e+02	1.27	1.72e+02	1.68e+03	1.20	0.018	0.002	9.45e-11
1	2	7.17e+01	6.17e+02	1.27	2.27e+02	2.65e+03	1.09	0.014	0.002	4.85e-08
2	0.2	1.27e+01	1.04e+03	1.11	3.11e+00	1.52e+04	1.00	0.009	0.002	-3.21e-09
2	1	1.27e+01	1.04e+03	1.11	2.79e+02	3.05e+04	1.20	0.021	0.003	1.17e-06
2	2	1.27e+01	1.04e+03	1.11	2.78e+02	3.84e+04	1.09	0.016	0.002	3.75e-04

In Table 1, we denote

$$\begin{aligned}\gamma_L &= \frac{a}{1 - c\varepsilon} / \|\tilde{L}\|_F, \quad \gamma_L(D_L) = \left(\|\tilde{L} D_L^{-1}\|_2 \|D_L \tilde{L}^{-1}\|_2 \right) \|\tilde{U}_{n-1}\|_F / \|\tilde{L}\|_F, \\ \gamma_U &= \frac{b}{1 + c\varepsilon} / \|\tilde{U}\|_F, \quad \gamma_U(D_U) = \left(\|D_U^{-1} \tilde{U}\|_2 \|\tilde{U} \tilde{U}^{-1} D_U\|_2 \right) \|\tilde{L}^{-1}\|_F / \|\tilde{U}\|_F, \\ \eta_{D_L} &= \|\tilde{L} D_L^{-1}\|_2 / \|\tilde{L} D_L^{-1}\|_2, \quad \eta_{D_U} = \|D_U^{-1} \tilde{U}\|_2 / \|D_U^{-1} \tilde{U}\|_2, \quad \tau = c\varepsilon,\end{aligned}$$

and t_γ and $t_{\gamma(D)}$ the time cost for computing γ_L, γ_U and $\gamma_L(D_L), \gamma_U(D_U)$, respectively.

Remark 3.5. Considering the definitions of the matrix norms used above, the fact that for any matrix $X \in \mathbb{R}^{n^2 \times n^2}$, $|M_{\text{uvec}} X| = M_{\text{uvec}} |X|$, $|M_{\text{svec}} X| = M_{\text{svec}} |X|$, $|M_{\text{ut}} X| = M_{\text{ut}} |X|$, $|M_{\text{slt}} X| = M_{\text{slt}} |X|$, (2.6), and (3.25), we can verify that the matrices M_{uvec} and M_{svec} in $Y_{\tilde{L}}$ and $Y_{\tilde{U}}$ involved in the bounds given above can be omitted. Thus, the bounds will become concise in form. However, the orders of the matrices in these bounds will increase from $v_1 \times n^2$ or $v_2 \times n^2$ to $n^2 \times n^2$.

4. PERTURBATION BOUNDS FOR THE QR FACTORIZATION

Assume that the matrices A , Q , and R in (1.2) are perturbed as

$$A \rightarrow A + \Delta A, \quad Q \rightarrow Q + \Delta Q, \quad R \rightarrow R + \Delta R,$$

where $\Delta A \in \mathbb{R}^{m \times n}$, $\Delta Q \in \mathbb{R}^{m \times n}$ is such that $(Q + \Delta Q)^T (Q + \Delta Q) = I_n$, and $\Delta R \in \mathbb{U}_n$. Thus, the perturbed QR factorization of A is

$$A + \Delta A = (Q + \Delta Q)(R + \Delta R). \quad (4.1)$$

Then

$$(R + \Delta R)^T (R + \Delta R) = (A + \Delta A)^T (A + \Delta A). \quad (4.2)$$

As done in Section 3, here the perturbation ΔR is also regarded as the unknown matrix. Expanding (4.2) and considering $A^T A = R^T R$ and (1.2) gives

$$R^T (\Delta R) + (\Delta R)^T R = R^T Q^T (\Delta A) + (\Delta A)^T Q R + (\Delta A)^T (\Delta A) - (\Delta R)^T (\Delta R).$$

Left-multiplying the above equation by R^{-T} and right-multiplying it by R^{-1} leads to

$$(\Delta R) R^{-1} + R^{-T} (\Delta R)^T = Q^T (\Delta A) R^{-1} + R^{-T} (\Delta A)^T Q + R^{-T} [(\Delta A)^T (\Delta A) - (\Delta R)^T (\Delta R)] R^{-1}.$$

Note that $(\Delta R)R^{-1}$ is upper triangular. Then using the operator ‘up,’ we have

$$(\Delta R)R^{-1} = \text{up} [Q^T(\Delta A)R^{-1} + R^{-T}(\Delta A)^T Q] + \text{up} (R^{-T} [(\Delta A)^T(\Delta A) - (\Delta R)^T(\Delta R)] R^{-1}).$$

Applying the operator ‘vec’ to the above equation and using (2.7), (2.4), and (2.8) yields

$$\begin{aligned} (R^{-T} \otimes I_n) \text{vec}(\Delta R) &= M_{\text{up}} [R^{-T} \otimes I_n + (I_n \otimes R^{-T}) \Pi_{nn}] \text{vec} [Q^T(\Delta A)] \\ &\quad + M_{\text{up}} (R^{-T} \otimes R^{-T}) \text{vec} [(\Delta A)^T(\Delta A) - (\Delta R)^T(\Delta R)], \end{aligned}$$

which together with (2.9) implies

$$\begin{aligned} \text{vec}(\Delta R) &= (R^T \otimes I_n) M_{\text{up}} [R^{-T} \otimes I_n + (I_n \otimes R^{-T}) \Pi_{nn}] \text{vec} [Q^T(\Delta A)] \\ &\quad + (R^T \otimes I_n) M_{\text{up}} (R^{-T} \otimes R^{-T}) \text{vec} [(\Delta A)^T(\Delta A) - (\Delta R)^T(\Delta R)]. \end{aligned} \quad (4.3)$$

Since ΔR is upper triangular, (2.4), (2.6), and (2.3) together gives

$$\text{vec}(\Delta R) = \text{vec}(\text{ut}(\Delta R)) = M_{\text{ut}} \text{vec}(\Delta R) = M_{\text{uvec}}^T M_{\text{uvec}} \text{vec}(\Delta R) = M_{\text{uvec}}^T \text{uvec}(\Delta R). \quad (4.4)$$

Substituting (4.4) into (4.3) and then premultiplying it by M_{uvec} and using (2.5), we have

$$\begin{aligned} \text{uvec}(\Delta R) &= M_{\text{uvec}} (R^T \otimes I_n) M_{\text{up}} [R^{-T} \otimes I_n + (I_n \otimes R^{-T}) \Pi_{nn}] \text{vec} [Q^T(\Delta A)] \\ &\quad + M_{\text{uvec}} (R^T \otimes I_n) M_{\text{up}} (R^{-T} \otimes R^{-T}) \text{vec} [(\Delta A)^T(\Delta A) - (\Delta R)^T(\Delta R)]. \end{aligned} \quad (4.5)$$

Conversely, left-multiplying (4.5) by M_{uvec}^T and considering (4.4) and (2.6), we obtain

$$\begin{aligned} \text{vec}(\Delta R) &= M_{\text{ut}} (R^T \otimes I_n) M_{\text{up}} [R^{-T} \otimes I_n + (I_n \otimes R^{-T}) \Pi_{nn}] \text{vec} (Q^T(\Delta A)) \\ &\quad + M_{\text{ut}} (R^T \otimes I_n) M_{\text{up}} (R^{-T} \otimes R^{-T}) \text{vec} [(\Delta A)^T(\Delta A) - (\Delta R)^T(\Delta R)]. \end{aligned}$$

From the definitions of M_{ut} and M_{up} , it is easy to check that $M_{\text{ut}} (R^T \otimes I_n) M_{\text{up}} = (R^T \otimes I_n) M_{\text{up}}$. Then the equation (4.3) is equivalent to (4.5).

As a matter of convenience, let

$$G_R = M_{\text{uvec}} (R^T \otimes I_n) M_{\text{up}} [R^{-T} \otimes I_n + (I_n \otimes R^{-T}) \Pi_{nn}], \quad H_R = M_{\text{uvec}} (R^T \otimes I_n) M_{\text{up}} (R^{-T} \otimes R^{-T}),$$

where G_R is equal to $W_R^{-1} Z_R$ in [12, Eqn. (3.4.2)], but the explicit expression for $W_R^{-1} Z_R$ was not provided in [12, 19]. The fact for equality can be derived from (4.5) and [12, Eqn. (3.4.2)] by setting $t = \varepsilon$ in [12, Eqn. (3.4.2)] and dropping the higher-order terms. Now, applying the operator ‘uvec[†]’ to (4.5) leads to

$$\Delta R = \text{uvec}^\dagger \left(G_R \text{vec} [Q^T(\Delta A)] + H_R \text{vec} [(\Delta A)^T(\Delta A) - (\Delta R)^T(\Delta R)] \right). \quad (4.6)$$

In the following, with the help of Lyapunov majorant function and the Banach fixed point principle, we develop the rigorous perturbation bounds for ΔR based on (4.6).

We first rewrite (4.6) as an operator equation for ΔR ,

$$\begin{aligned} \Delta R &= \Psi(\Delta R, Q^T(\Delta A), \Delta A) \\ &= \text{uvec}^\dagger \left(G_R \text{vec} [Q^T(\Delta A)] + H_R \text{vec} [(\Delta A)^T(\Delta A) - (\Delta R)^T(\Delta R)] \right). \end{aligned} \quad (4.7)$$

Assuming that $Z \in \mathbb{U}_n$ and replacing ΔR in (4.7) with Z leads to

$$Z = \Psi(Z, Q^T(\Delta A), \Delta A), \quad (4.8)$$

where $\Psi(Z, Q^T(\Delta A), \Delta A) = \text{uvec}^\dagger \left(G_R \text{vec} \left(Q^T(\Delta A) \right) + H_R \text{vec} \left((\Delta A)^T(\Delta A) - Z^T Z \right) \right)$. Let $\|Z\|_F \leq \rho$ for some $\rho \geq 0$, $\|Q^T(\Delta A)\|_F = \delta_1$, and $\|\Delta A\|_F = \delta_2$. Then, noting (2.1),

$$\|\Psi(Z, Q^T(\Delta A), \Delta A)\|_F \leq \|G_R\|_2 \delta_1 + \|H_R\|_2 \delta_2^2 + \|H_R\|_2 \rho^2.$$

Thus, setting $\delta = \begin{bmatrix} \delta_1 \\ \delta_2 \end{bmatrix}$, we have the Lyapunov majorant function of the operator equation (4.8)

$$h(\rho, \delta) = a\delta_1 + b\delta_2^2 + b\rho^2,$$

where $a = \|G_R\|_2$ and $b = \|H_R\|_2$. Then the Lyapunov majorant equation is

$$h(\rho, \delta) = \rho, \text{ i.e., } a\delta_1 + b\delta_2^2 + b\rho^2 = \rho. \quad (4.9)$$

Assuming that $\delta \in \Omega = \{\delta_1 \geq 0, \delta_2 \geq 0 : 1 - 4b(a\delta_1 + b\delta_2^2) \geq 0\}$, we have two solutions to the Lyapunov majorant equation (4.9): $\rho_1(\delta) \leq \rho_2(\delta)$ with

$$\rho_1(\delta) := f_1(\delta) := \frac{2(a\delta_1 + b\delta_2^2)}{1 + \sqrt{1 - 4b(a\delta_1 + b\delta_2^2)}}.$$

Let the set $\mathcal{B}(\delta)$ be

$$\mathcal{B}(\delta) = \{Z \in \mathbb{U}_n : \|Z\|_F \leq f_1(\delta)\} \subset \mathbb{R}^{n \times n}.$$

It is closed and convex. In this case, the operator $\Psi(\cdot, Q^T(\Delta A), \Delta A)$ maps the set $\mathcal{B}(\delta)$ into itself. Furthermore, when $\delta \in \Omega_1 = \{\delta_1 \geq 0, \delta_2 \geq 0 : 1 - 4b(a\delta_1 + b\delta_2^2) > 0\}$, we have that the derivative of the function $h(\rho, \delta)$ relative to ρ at $f_1(\delta)$ satisfies

$$h'_\rho(f_1(\delta), \delta) = 1 - \sqrt{1 - 4b(a\delta_1 + b\delta_2^2)}\rho < 1.$$

Meanwhile, for $Z, \tilde{Z} \in \mathcal{B}(\delta)$,

$$\|\Psi(Z, Q^T(\Delta A), \Delta A) - \Psi(\tilde{Z}, Q^T(\Delta A), \Delta A)\|_F \leq h'_\rho(f_1(\delta), \delta) \|Z - \tilde{Z}\|_F.$$

The above facts mean that the operator $\Psi(\cdot, Q^T(\Delta A), \Delta A)$ is contractive on the set $\mathcal{B}(\delta)$ when $\delta \in \Omega_1$. According to the Banach fixed point principle, the operator equation (4.8) has a unique solution in the set $\mathcal{B}(\delta)$ for $\delta \in \Omega_1$, and so do the operator equation (4.7) and then the matrix equation (4.2). Then $\|\Delta R\|_F \leq f_1(\delta)$ for $\delta \in \Omega_1$. In this case, the unknown matrix ΔQ in (4.1) is also determined uniquely.

The above discussions implies another main theorem.

Theorem 4.1. *Let the unique QR factorization of $A \in \mathbb{R}_n^{m \times n}$ be as in (1.2) and $\Delta A \in \mathbb{R}^{m \times n}$. If*

$$\|H_R\|_2 \left(\|G_R\|_2 \|\Delta A\|_F + \|H_R\|_2 \|\Delta A\|_F^2 \right) < \frac{1}{4}, \quad (4.10)$$

then $A + \Delta A$ has the unique QR factorization (4.1) and

$$\|\Delta R\|_F \leq \frac{2 \left(\|G_R\|_2 \|Q^T(\Delta A)\|_F + \|H_R\|_2 \|\Delta A\|_F^2 \right)}{1 + \sqrt{1 - 4 \|H_R\|_2 \left(\|G_R\|_2 \|Q^T(\Delta A)\|_F + \|H_R\|_2 \|\Delta A\|_F^2 \right)}} \quad (4.11)$$

$$\leq 2 \left(\|G_R\|_2 \|Q^T(\Delta A)\|_F + \|H_R\|_2 \|\Delta A\|_F^2 \right) \quad (4.12)$$

$$< (1 + 2 \|G_R\|_2) \|\Delta A\|_F. \quad (4.13)$$

Proof. It is easy to see that the condition (4.10) is more constraining than the one in Ω_1 . Thus, from the discussions before Theorem 4.1, we derive all results in Theorem 4.1 except the bound (4.13).

After some computations, from (4.10), it follows that

$$2 \|H_R\|_2 \|\Delta A\|_F < \sqrt{1 + \|G_R\|_2^2} - \|G_R\|_2. \quad (4.14)$$

Substituting (4.14) into (4.12) and noting $\|Q^T(\Delta A)\|_F \leq \|\Delta A\|_F$ gives

$$\|\Delta R\|_F < \left(\sqrt{1 + \|G_R\|_2^2} + \|G_R\|_2 \right) \|\Delta A\|_F.$$

Using the fact $\sqrt{1 + \|G_R\|_2^2} \leq 1 + \|G_R\|_2$, we have the bound (4.13). \square

Remark 4.1. According to (4.14), the condition (4.10) can be simplified and strengthened to

$$\|H_R\|_2 (1 + 2 \|G_R\|_2) \|\Delta A\|_F < \frac{1}{2}. \quad (4.15)$$

Remark 4.2. The following first-order perturbation bound can be derived from (4.11) or (4.5) by omitting the higher-order terms

$$\|\Delta R\|_F \leq \|G_R\|_2 \|Q^T(\Delta A)\|_F + \mathcal{O}(\|\Delta A\|_F^2) \quad (4.16)$$

under the condition

$$\|A^\dagger\|_2 \|\Delta A\|_F < 1,$$

which ensures that the unique QR factorization of $A + \Delta A$ exists [12, 19].

The bound (4.16) without explicit expression was also derived in [19] by the matrix-vector equation approach, which is regarded as the optimal first-order bound for the triangular factor R [12, 19].

Remark 4.3. In [23], the following rigorous perturbation bound was derived by the combination of the classic and refined matrix equation approaches,

$$\|\Delta R\|_F \leq (\sqrt{6} + \sqrt{3}) \left(\inf_{D \in \mathbb{D}_n} \sqrt{1 + \zeta_D^2} k_2(D^{-1}R) \right) \|\Delta A\|_F, \quad (4.17)$$

under the condition

$$\|A^\dagger\|_2 \|\Delta A\|_F < \sqrt{3/2} - 1. \quad (4.18)$$

In (4.17), $D = \text{diag}(\delta_1, \delta_2, \dots, \delta_n)$ and $\zeta_D = \max_{1 \leq i < j \leq n} (\delta_j / \delta_i)$. The discussions in [23] shows that the bound (4.17) can be much tighter than the previous one derived by the classic matrix equation approach. From [19, Eqns. (5.19) and (5.20)] and the fact $G_R = W_R^{-1} Z_R$ mentioned above, we have

$$1 \leq \|G_R\|_2 \leq \inf_{D \in \mathbb{D}_n} \sqrt{1 + \zeta_D^2} k_2(D^{-1}R), \quad (4.19)$$

which indicates that the bound (4.13) is tighter than (4.17).

Using the expression of H_R and the definitions of M_{uvec} and M_{up} , we obtain

$$\|H_R\|_2 \geq \|R^{-1}\|_2 / 2 = \|A^\dagger\|_2 / 2, \quad (4.20)$$

which together with the first inequality in (4.19) suggests that

$$\|H_R\|_2(1 + 2\|G_R\|_2)\|\Delta A\|_F \geq \frac{3}{2}\|A^\dagger\|_2\|\Delta A\|_F.$$

The above inequality is approximately attainable since the inequality (4.20) and the first inequality in (4.19) are attainable and approximately attainable [12, 19], respectively. Moreover, $1/3 > \sqrt{3/2} - 1$. So, although the strengthened condition (4.15) may be more constraining than (4.18), the former is not so strong. In addition, it should be mentioned that it is more expensive to estimate the bound (4.13) than that of (4.17) since the matrix G_R involved in the former contains the Kronecker products.

In the following, we consider the rigorous perturbation bounds for the triangular factor R of the QR factorization when the perturbation ΔA has the form of backward error resulting from the standard QR factorization algorithm. That is, $\Delta A \in \mathbb{R}^{m \times n}$ satisfies (see, e.g., [2, 3, 18, 20]),

$$|\Delta A| \leq \varepsilon C|A|, \quad (4.21)$$

where $C = (c_{ij}) \in \mathbb{R}^{m \times m}$, $0 \leq c_{ij} \leq 1$, and $\varepsilon \geq 0$ is a small constant. In this case,

$$\begin{aligned} \|\Psi(Z, Q^T(\Delta A), \Delta A)\|_F &\leq \| |G_R| \text{vec}(|Q^T|C|Q||R|) \|_F \varepsilon + \| |H_R| \text{vec}(|R^T||Q^T|C^T C|Q||R|) \|_F \varepsilon^2 \\ &\quad + \| |H_R| \|_2 \rho^2 \\ &\leq \| |G_R| |R^T| \otimes I_n \|_2 \| |Q^T|C|Q| \|_F \varepsilon + \| |H_R| |R^T| \otimes |R^T| \|_2 \| |Q^T|C^T C|Q| \|_F \varepsilon^2 \\ &\quad + \| |H_R| \|_2 \rho^2. \end{aligned} \quad (4.22)$$

From (4.22), we have the Lyapunov majorant function of the operator equation (4.8) and then (4.7),

$$h(\rho, \varepsilon) = \tilde{a}\varepsilon + \tilde{b}\varepsilon^2 + \tilde{c}\rho^2,$$

where

$$\tilde{a} = \| |G_R| |R^T| \otimes I_n \|_2 \| |Q^T|C|Q| \|_F,$$

and

$$\tilde{b} = \| |H_R| |R^T| \otimes |R^T| \|_2 \| |Q^T|C^T C|Q| \|_F, \quad \tilde{c} = \| |H_R| \|_2.$$

Then the Lyapunov majorant equation is

$$h(\rho, \varepsilon) = \rho, \text{ i.e., } \tilde{a}\varepsilon + \tilde{b}\varepsilon^2 + \tilde{c}\rho^2 = \rho.$$

Similar to the discussions before Theorem 4.1, we have that when $\varepsilon \in \Omega_1$, where

$$\Omega_1 = \left\{ \varepsilon \geq 0 : 1 - 4\tilde{c}(\tilde{a}\varepsilon + \tilde{b}\varepsilon^2) > 0 \right\},$$

the operator equations (4.8) and (4.7), i.e., the matrix equation (4.2), has a unique solution in the set

$$\mathcal{B}(\varepsilon) = \{Z \in \mathbb{U}_n : \|Z\|_F \leq f_1(\varepsilon)\} \subset \mathbb{R}^{n \times n},$$

where $f_1(\varepsilon) := \frac{2(\tilde{a}\varepsilon + \tilde{b}\varepsilon^2)}{1 + \sqrt{1 - 4\tilde{c}(\tilde{a}\varepsilon + \tilde{b}\varepsilon^2)}}$. Then $\|\Delta R\|_F \leq f_1(\varepsilon)$ for $\varepsilon \in \Omega_1$. In this case, the unknown matrix ΔQ in (4.1) is also determined uniquely.

In summary, we have the following theorem.

Theorem 4.2. *Let the unique QR factorization of $A \in \mathbb{R}_n^{m \times n}$ be as in (1.2) and $\Delta A \in \mathbb{R}^{m \times n}$ be a perturbation matrix in A such that (4.21) holds. If*

$$\tilde{c}(\tilde{a}\varepsilon + \tilde{b}\varepsilon^2) < \frac{1}{4}, \quad (4.23)$$

then $A + \Delta A$ has the unique QR factorization (4.1) and

$$\|\Delta R\|_F \leq \frac{2(\tilde{a}\varepsilon + \tilde{b}\varepsilon^2)}{1 + \sqrt{1 - 4\tilde{c}(\tilde{a}\varepsilon + \tilde{b}\varepsilon^2)}} \quad (4.24)$$

$$\leq 2 \|G_R\|_2 \|R^T \otimes I_n\|_2 \|Q^T |C| Q\|_F \varepsilon + 2 \|H_R\|_2 \|R^T \otimes |R^T|\|_2 \|Q^T |C^T C| Q\|_F \varepsilon^2 \quad (4.25)$$

$$< \left(\|R\|_2 \|C|Q\|_F + 2 \|G_R\|_2 \|R^T \otimes I_n\|_2 \|Q^T |C| Q\|_F \right) \varepsilon. \quad (4.26)$$

Proof. Obviously, we only need to show that the bound (4.26) holds. To see it, we only note the fact

$$0 \leq 2\tilde{b}\varepsilon < \sqrt{\tilde{b}/\tilde{c} + \tilde{a}^2} - \tilde{a} \leq (\tilde{b}/\tilde{c})^{1/2} \leq \|R\|_2 \|C|Q\|_F, \quad (4.27)$$

which can be derived from (4.23) and (2.1). \square

Remark 4.4. Using (4.27), the condition (4.23) can be simplified and strengthened to

$$\|H_R\|_2 \left(\|R\|_2 \|C|Q\|_F + 2 \|G_R\|_2 \|R^T \otimes I_n\|_2 \|Q^T |C| Q\|_F \right) \varepsilon < \frac{1}{2}. \quad (4.28)$$

Remark 4.5. From (4.24), we have the following first-order perturbation bound

$$\|\Delta R\|_F \leq \|G_R\|_2 \|R^T \otimes I_n\|_2 \|Q^T |C| Q\|_F \varepsilon + \mathcal{O}(\varepsilon^2). \quad (4.29)$$

Replacing G_R with $W_R^{-1} Z_R$ in (4.29) gives the optimal first-order perturbation bound derived by the matrix-vector equation approach in [18, Eqn. (8.5)]. In addition, the condition for the bound (4.29) to hold, i.e., for the unique QR factorization $A + \Delta A$ to exist [24], is

$$\|R\|_2 \|R^{-1}\|_2 \|C|Q\|_F \varepsilon < 1.$$

Remark 4.6. The following rigorous perturbation bound was derived by the combination of the classic and refined matrix equation approaches in [23, 24],

$$\|\Delta R\|_F \leq (\sqrt{6} + \sqrt{3}) \left(\inf_{D \in \mathbb{D}_n} \sqrt{1 + \zeta_D^2} \|D^{-1} R\|_2 \|R\|_2 \|R^{-1} D\|_2 \right) \|C|Q\|_F \varepsilon, \quad (4.30)$$

under the condition

$$\|R\|_2 \|R^{-1}\|_2 \|C|Q\|_F \varepsilon < \sqrt{3/2} - 1. \quad (4.31)$$

It should be claimed that the bound (4.30) is a little different from the one in [23, 24]. From the discussions in [24], we know that the bound (4.30) can be much smaller than the one in [18, Section 6]. Using (2.1), it is seen that $\|Q^T |C| Q\|_F \leq \|Q\|_2 \|C|Q\|_F$. Meanwhile, from [18, Eqns. (8.11) and (8.10), and an equation above (8.7)] and the fact $G_R = W_R^{-1} Z_R$, it follows that

$$\|R\|_2 \leq \|G_R\|_2 \|R^T \otimes I_n\|_2 \leq \inf_{D \in \mathbb{D}_n} \sqrt{1 + \zeta_D^2} \|D^{-1} R\|_2 \|R\|_2 \|R^{-1} D\|_2. \quad (4.32)$$

Thus, when $\|Q\|_2 = 1$ and $\|D^{-1}R\|_2 = \|D^{-1}R\|_2$, the bound (4.26) will be tighter than (4.30). As explained in Remark 3.4, a suitable scaling matrix D can make the difference between $\|D^{-1}R\|_2$ and $\|D^{-1}R\|_2$ be unremarkable. See the following examples. So, if $\|Q\|_2 = 1$, the bound (4.26) is usually tighter than (4.30). See Example 4.1 below. Otherwise, since $\|Q^T|C|Q\|_F$ is at most $\|Q\|_2$ times as large as $\|C|Q\|_F$, in general, the fact (4.32) indicates that the bound (4.26) still has advantages. See Example 4.2 below. In addition, we note that the difference between $\|Q^T|C|Q\|_F$ and $\|C|Q\|_F$ may increase as the order n of the involved matrix increases. Example 4.2 given below shows that, in this case, the bound (4.26) still behaves good.

Whereas, the strengthened condition (4.28) may be more constraining than the one (4.31) owing to the first inequality in (4.32) and $\|H_R\|_2 \geq \|R^{-1}\|_2/2$. It is worthy pointing out that the two inequalities mentioned above are attainable [18]. Meanwhile, it is more expensive to estimate the bound (4.26) than that of (4.30), especially when n is large.

In the following examples, as done in [18], we choose the scaling matrix D_r defined by $D_r = \text{diag}(\|R(j, :)\|_2)$ and the scaling matrix $D_e = \text{diag}(\delta_1, \delta_2, \dots, \delta_n)$ defined as follows: $\delta_1 = 1/\|(D_c R^{-1})(:, 1)\|_2$; for $j = 2, 3, \dots, n$: $\delta_j = 1/\|(D_c R^{-1})(:, j)\|_2$ if $\|(D_c R^{-1})(:, j)\|_2 \geq \|(D_c R^{-1})(:, j-1)\|_2$, otherwise, $\delta_j = \delta_{j-1}$. Here $D_c = \text{diag}(\|R(j, :)\|_1)$. More on methods and explanations of choosing the scaling matrix can be found in [12] or [14]. In Tables 2–4, we denote

$$q = \|Q^T|C|Q\|_F / \|C|Q\|_F, \quad \gamma_R = (\|R\|_2 \|C|Q\|_F + 2 \|G_R\|_2 \|Q^T|C|Q\|_F) / \|R\|_2, \\ \gamma_R(X) = (\sqrt{6} + \sqrt{3}) \left(\sqrt{1 + \zeta_X^2} \|X^{-1}R\|_2 \|R\|_2 \right) \|C|Q\|_F / \|R\|_2, \quad \eta_X = \|X^{-1}R\|_2 / \|X^{-1}R\|_2,$$

where $X = D_r$ or D_e , and t_Y the time cost for computing the estimate Y . One more statement is that the testing environment is the same as that of Example 3.1.

Example 4.1. This example is from [18]. That is, the test A is the $n \times n$ Kahan matrix:

$$A = \text{diag}(1, s, s^2, \dots, s^{n-1}) \begin{bmatrix} 1 & -c & \cdots & -c \\ & 1 & \cdots & -c \\ & & \ddots & \vdots \\ & & & 1 \end{bmatrix},$$

where $c = \cos(\theta)$ and $s = \sin(\theta)$. In this case, $R = A$ and $Q = I_n$. Obviously, $\|Q\|_2 = 1$. The numerical results for $n = 5, 10, 15, 20, 25$ with $\theta = \pi/8$ and the corresponding random matrix C produced by the MATLAB function **rand** are shown in Table 2, which indicate the expectation claimed in Remark 4.6.

Table 2: Comparison of rigorous bounds for the $n \times n$ Kahan matrix

n	γ_R	t_{γ_R}	$\gamma_R(D_r)$	$t_{\gamma_R(D_r)}$	η_{D_r}	$\gamma_R(D_e)$	$t_{\gamma_R(D_e)}$	η_{D_e}
5	4.10e+01	0.003	1.66e+02	0.001	1.27	1.79e+02	0.001	1.05
10	1.48e+03	0.010	9.00e+03	0.001	1.27	1.05e+04	0.001	1.03
15	4.38e+04	0.036	3.43e+05	0.002	1.21	3.91e+05	0.002	1.03
20	1.35e+06	0.190	1.26e+07	0.002	1.16	1.40e+07	0.004	1.03
25	3.87e+07	0.673	4.15e+08	0.004	1.13	4.54e+08	0.004	1.03

Example 4.2. Each test matrix has the same form as the one in Example 3.1. The numerical results for $n = 20$, $d_1, d_2 \in \{0.8, 1, 2\}$, the same random matrix B produced by the MATLAB function **randn**,

and the same random matrix C produced by the MATLAB function **rand** are shown in Table 3; the numerical results for $n = 20, 25, 30, 35, 40, 45, 50, 55$ with $d_1 = d_2 = 0.8$ and the corresponding random matrices B and C produced by the MATLAB functions **randn** and **rand**, respectively, are shown in Table 4. These results demonstrate the conjectures claimed in Remark 4.6.

Table 3: Comparison of rigorous bounds for $A = D_1 B D_2$

d_1	d_2	q	γ_R	t_{γ_R}	$\gamma_R(D_r)$	$t_{\gamma_R(D_r)}$	η_{D_r}	$\gamma_R(D_e)$	$t_{\gamma_R(D_e)}$	η_{D_e}
0.8	0.8	2.91	3.42e+02	0.191	1.50e+03	0.005	1.18	1.45e+03	0.003	1.00
0.8	1	2.91	9.73e+03	0.192	5.44e+04	0.003	1.21	4.50e+04	0.003	1.00
0.8	2	2.91	2.29e+04	0.187	2.90e+05	0.002	1.07	1.06e+05	0.003	1.00
1	0.8	3.49	4.50e+02	0.188	1.39e+03	0.003	1.15	1.32e+03	0.003	1.00
1	1	3.49	1.52e+04	0.189	6.62e+04	0.002	1.32	4.82e+04	0.003	1.00
1	2	3.49	2.38e+04	0.190	6.49e+05	0.003	1.12	7.56e+04	0.003	1.00
2	0.8	2.00	4.38e+02	0.187	3.77e+03	0.003	1.15	3.11e+03	0.003	1.02
2	1	2.00	3.39e+02	0.191	1.37e+05	0.003	1.17	2.33e+04	0.006	1.03
2	2	2.00	8.02e+03	0.188	1.94e+06	0.003	1.05	5.48e+04	0.002	1.00

Table 4: Comparison of rigorous bounds for $A = D_1 B D_2$ with $d_1 = d_2 = 0.8$

n	q	γ_R	t_{γ_R}	$\gamma_R(D_r)$	$t_{\gamma_R(D_r)}$	η_{D_r}	$\gamma_R(D_e)$	$t_{\gamma_R(D_e)}$	η_{D_e}
20	2.99	4.56e+02	0.190	1.24e+03	0.007	1.19	1.51e+03	0.009	1.08
25	3.22	8.42e+02	0.662	1.96e+03	0.005	1.10	2.39e+03	0.005	1.20
30	3.33	7.64e+02	1.914	2.93e+03	0.007	1.27	3.26e+03	0.006	1.05
35	3.31	7.29e+02	4.688	1.68e+03	0.008	1.22	3.05e+03	0.008	1.06
40	3.34	1.11e+03	10.69	3.06e+03	0.011	1.15	4.50e+03	0.009	1.14
45	3.45	1.04e+03	21.35	3.48e+03	0.013	1.18	4.69e+03	0.012	1.07
50	3.50	7.33e+02	39.81	2.65e+03	0.012	1.12	4.31e+03	0.012	1.00
55	3.46	1.51e+03	69.81	3.93e+03	0.014	1.28	6.75e+03	0.014	1.13

Remark 4.7. As done in the proof of Theorem 3.1 and Remark 3.5 and noting the fact $M_{\text{ut}}(R^T \otimes I_n)M_{\text{up}} = (R^T \otimes I_n)M_{\text{up}}$, we can check that the matrix M_{uvec} in G_R and H_R involved in the bounds given in this section can be omitted. In this case, the forms of these bounds will become concise, however, the orders of the matrices in these bounds will increase.

5. CONCLUDING REMARKS

In this paper, we propose a new approach to present the rigorous perturbation analysis for the LU and QR factorizations, and obtain new rigorous perturbation bounds with explicit expressions, which improve the previous ones in [23] and [24]. As the special case, the optimal first-order perturbation bounds with explicit expressions for the two factorizations are also given. The new approach can also be used to derive the rigorous perturbation bounds for the Cholesky factorization and the Cholesky downdating problem [11, 12, 30]. The derived bounds for the Cholesky factorization are the same as the ones in [11, 12] obtained by the combination of the matrix-vector equation approach and Theorem 3.1 in [25], but have the explicit expressions. Actually, noting the conditions and proof of Theorem 3.1 in [25], we find that the approach in [11, 12] can be regarded as a special case of the approach in this

paper. Furthermore, the new approach can also be generalized to apply the block matrix factorizations such as the block LU, SR, and Cholesky-like factorizations [31].

Although the explicit expressions of the new rigorous perturbation bounds and the optimal first-order perturbation bounds are provided, it is still expensive to estimate these bounds directly as the spectral norm of the large sparse matrices is involved. To reduce the computational cost, we can use the fact that, for any matrix X , $\|X\|_2^2 \leq \|X\|_1 \|X\|_\infty$. However, in this case, the bounds will be weakened. In addition, some techniques on sparse matrix (see e.g., [32]) may be used to overcome the above difficulties. We will consider this topic in the near future.

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